QAGC SUBMISSION

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REPLY SIGMA

OUTLINE

The algorithm is based on this paper [1]

1. General overview of [1]
2. Differences
3. Results

[1] Kishor Bharti, Tobias Haug. Iterative Quantum Assisted Eigensolver (2020) arXiv:2010.05638

ITERATIVE QUANTUM ASSISTED EIGENSOLVER

Let be the H Hamiltonian of interest and ψ its ground state
In general one cannot directly diagonalize H due to the exponential size of the Hilbert space.

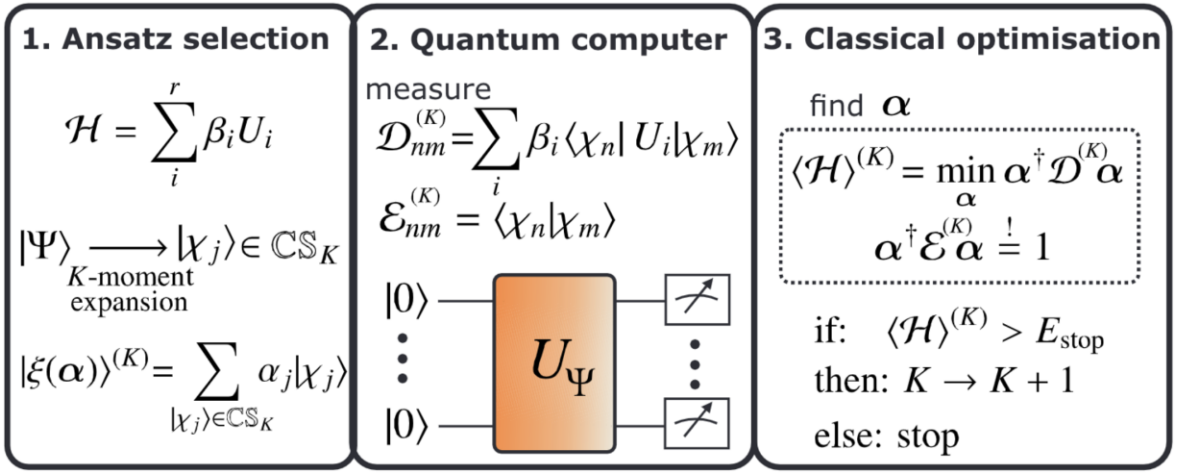
The idea is to create a subspace on which the Hamiltonian is diagonalized:

$$\psi = \sum_i \alpha_i \chi_i \qquad H\psi = E\psi \implies D\boldsymbol{\alpha} = ES\boldsymbol{\alpha}$$

$$\text{with} \quad D_{i,j} = \langle \psi_i | H | \psi_j \rangle \quad \text{and} \quad S_{i,j} = \langle \psi_i | \psi_j \rangle$$

ITERATIVE QUANTUM ASSISTED EIGENSOLVER

Now one can choose any subspace basis $\{\chi_i\}_i^k$, compute the matrix elements on a quantum computer and solve the generalized eigenvalue problem $D\boldsymbol{\alpha} = ES\boldsymbol{\alpha}$ on a classical one.



CHOICE OF SUBSPACE

Let $H = \sum_i U_i$ and some initial state $|\psi_0\rangle$
One possible basis for the subspace is to take states of the form $|\chi_j\rangle = U_{i_1} \cdots U_{i_k}|\psi_0\rangle \equiv O_j|\psi_0\rangle$

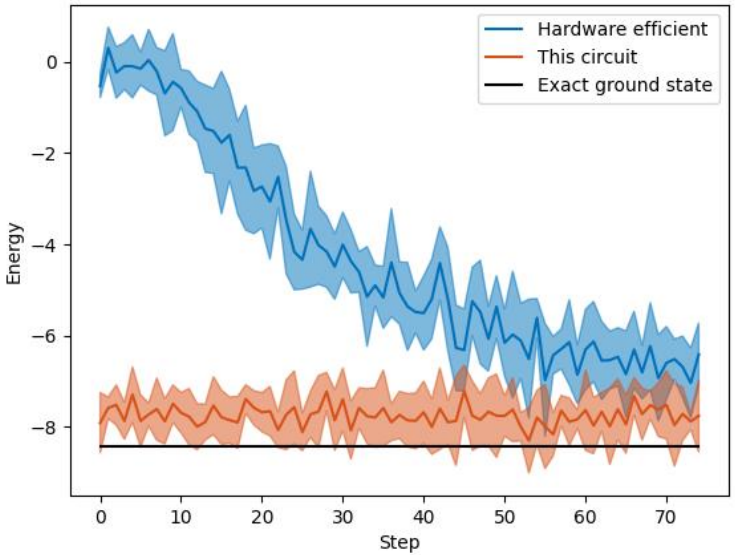
The main advantage is that all matrix elements are expectation values over ψ_0 of some operators: $O_i^\dagger O_j$ for $S_{i,j}$ and $O_i^\dagger H O_j$ for $D_{i,j}$

In our case, U_i are Pauli words

And the starting state $|\psi_0\rangle$ is the result of a VQE

VQE

The VQE ansatz chosen is based on a selection of single excitations implemented as Givens rotations from the Jordan-Wigner Hamiltonian representation



The energies as a function of the step of the VQE are shown for this Ansatz and for the hardware efficient Ansatz as a comparison. This is done for 8 qubits, with noise.

This result lead us to use only few steps for the VQE, leaving us more QPU time for the rest of the algotrithm

DIFFERENCIES

Because of the QPU time constraint, only a small basis can be used, and no iteration over the basis are done.
Here, only a subspace of size 2 is considered. The basis is composed of $|\psi_0\rangle$ since it is already a good approximation of the ground state, and another element, chosen as such : we take the Pauli word of H with the highest coefficient, that contain at least 4 pauli X or Y operators (in order to have a small overlap with $|\psi_0\rangle$)

Next, because of the error on the state preparation $|\psi_0\rangle$, the noise on the gates and the statistical error on the measurement, the result of the generalized eigendecomposition is quite unstable.
To overcome this, multiple diagonalisations are done, and only energies close to the results of the VQE are kept. This avoid outliers, but can also limit the accuracy.

RESULTS AND IMPROVEMENTS

From the sample that we computed, the absolute error of the energy is 0.25 in average, with a high standart deviation of 0.25 as well.
The error range from 1 to 2e-3, giving between 1 and 500 points.
However, the points are computed by the inverse of the **mean** of the absolute error over three runs.
Therefore, the score it is very sensitive to the worst case.

An improvement would be to have a more stable way to use the subspace diagonaliation with noise on the matrix elements

We could also improve the Hamiltonian terms grouping (not only to qwc terms) and work out with basis for co-diagonalisation